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Viral genome structures, charge, and sequences are optimal for capsid assembly[1]

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For many viruses, the spontaneous assembly of a capsid shell around the nu-cleic acid (NA) genome is an essential step in the viral life cycle. Capsid formation is a multicomponent, out-of-equilibrium assembly process for which kinetic effects and thermodynamic constraints compete to determine the outcome. Understand-ing how viral components drive highly efficient assembly under these constraints could promote biomedical efforts to block viral propagation, and would elucidate the factors controlling assembly in a wide range of systems containing proteins and polyelectrolytes. This talk will describe coarse-grained models of capsid proteins and NAs with which we investigate the dynamics and thermodynamics of virus assembly. In con-trast to recent theoretical models, we find that capsids spontaneously 'overcharge'; that is, the NA length which is kinetically and thermodynamically optimal possess-es a negative charge greater than the positive charge of the capsid. When applied to specific virus capsids, the calculated optimal NA lengths closely correspond to the natural viral genome lengths. These results suggest that the features included in this model (i.e. electrostatics, excluded volume, and NA tertiary structure) play key roles in determining assembly thermodynamics and consequently exert selec-tive pressure on viral evolution. I will then discuss mechanisms by which se-quence-specific interactions between NAs and capsid proteins promote selective encapsidation of the viral genome.

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